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The Essential Self-Adjointness of Generalized Schrödinger Operators

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A necessary and sufficient condition is given for the generalized Schrödinger operator $A = -(1/2\rho) \sum_{i=1}^{n} D_i(\rho D_i)$ to be essentially self-adjoint in $L^2(\Omega; \rho\, dx)$, under general assumptions on ρ and for arbitrary domains Ω in $\mathbb{R}^n$. In particular, if ρ is strictly positive and locally Lipschitz continuous on $\Omega = \mathbb{R}^n$, then A is essentially self-adjoint. Examples of non-essential self-adjointness and a complete discussion of the one-dimensional case are also given. These results have applications to the problem of the essential self-adjointness of quantum Hamiltonians and to the uniqueness problem of Markov processes.

0. INTRODUCTION

The essential self-adjointness of second-order elliptic operators has been studied extensively; for a survey of known results see. e.g., [15] and the references therein. Recently, some attention was paid to the problem of the essential self-adjointness of the differential operator $A = -(1/2\rho) \sum_{i=1}^{n} D_i(\rho D_i)$ in the Hilbert space $L^2(\mathbb{R}^n; \rho\, dx)$, where ρ is a given function, positive almost everywhere on $\mathbb{R}^n$ ([3, 4, 12, 26]).

An important feature of A is its unitary equivalence to some Schrödinger operator H; in fact, setting $\phi = \sqrt{\rho}$,

$$\begin{aligned} H &= \phi A \phi^{-1} \\ &= -\frac{1}{2}\Delta + V \qquad \text{with} \quad V = \frac{1}{2}\frac{\Delta\phi}{\phi} \end{aligned} \tag{0.1}$$

defines a symmetric operator in $L^2(\mathbb{R}^n; dx)$, which is unitary equivalent to A.

Conversely, let $H = -\frac{1}{2}\Delta + V$ be a Schrödinger operator in $L^2(\mathbb{R}^n; dx)$ with lower bounded spectrum $Sp(H)$ and let $E = \inf Sp(H)$ be an eigenvalue

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of H. Then the relation (0.1) holds, if we replace the potential V by $V-E$ and take the positive eigenfunction of 0 (the ground state) as the functions ϕ.

Hence, the study of lower bounded Schrödinger operators is in a good sense equivalent to the study of the operator A. This observation essentially originates from the approach to quantum mechanics and quantum field theory by the theory of Dirichlet forms, see, e.g. [4–6, 11, 24]. The basic use is to define quantum Hamiltonians (and hence the quantum dynamics) in cases where the potential V is more general than a measurable function ([4, 24]). This is the reason why A is called a "generalized Schrödinger operator" ([10]).

The essential self-adjointness of the operators A and H has important probabilistic implications: In general, A has several self-adjoint extensions A' giving rise to Markov processes with transition semigroups $p_t = e^{-tA'}$. The essential self-adjointness of A implies that there is only one such semigroup, hence a unique Markov process with a generator extending A. On the other hand, the essential self-adjointness of H, as defined by $\phi A \phi^{-1}$, has the analytic consequence of the uniqueness of the quantum dynamics defined by H.

In the above-mentioned papers, Albeverio, Hoegh-Krohn and Streit ([4]) and Hooton ([12]) used the relation (0.1) as a convenient tool to prove the essential self-adjointness of A. But for the operator H being well-defined and essentially self-adjoint in $L^2(\mathbb{R}^n; dx)$, smoothness and growth type assumptions on the function ρ are needed. Moreover, this procedure involves a dependence of the domain $\mathscr{D}(A)$ of A on ρ. This causes problems, if one wants to extend these methods to the infinite dimensional case, where $\mathbb{R}^n$ is replaced by some Banach or Hilbert space (see, e.g. [1, 2, 17]).

In this paper, we treat the question of the essential self-adjointness of the generalized Schrödinger operator A directly. In contrast with the previous results, our assumptions do not involve any smoothness of ρ; in fact, they allow to control Schrödinger operators with singular or distributional potentials (Example 2.9).

The next paragraph will be a brief summary of the content of this paper.

Throughout this paper, Ω is a domain in $\mathbb{R}^n$ and $\rho: \Omega \to \mathbb{R}$ is a function with the following properties:

$$\rho(x) > 0 \text{ for Lebesgue-a.e. } x \in \Omega,\ \rho \text{ is weakly differentiable, } D_i\rho/\rho \in L^2_{\mathrm{loc}}(\Omega; \rho\, dx) \text{ for } 1 \leqslant i \leqslant n, \text{ where } D_i\rho \text{ denotes the weak derivative of } \rho \text{ with respect to the } x_i\text{-axis.} \tag{0.2}$$

Then, the generalized Schrödinger operator A, defined on the domain $\mathscr{D}(A) = \mathscr{C}_0^\infty(\Omega)$, is symmetric and nonnegative definite in the Hilbert space $L^2(\Omega; \rho\, dx)$. Hence, there exist self-adjoint extensions of A and A is essentially self-adjoint, if it has only one self-adjoint extension. In this paper, we use as a basic tool the following criterion ([19, Theorem X.26]):

A is essentially self-adjoint iff the adjoint operator A^* satisfies the condition $\operatorname{Ker}(A^* + \alpha) := \{f \in \mathscr{D}(A^*) \mid A^*f + \alpha f = 0\} = \{0\}$ for any $\alpha > 0$. (0.3)

In the first section, we construct two distinguished self-adjoint extensions of A. We use them to establish a criterion for the essential self-adjointness of A in terms of their associated closed bilinear forms (Theorem 1.3). In the case $\Omega \neq \mathbb{R}^n$, this criterion yields an easy method to find examples where A is not essentially self-adjoint.

In the second section, we are concerned with the one-dimensional case; i.e., $\Omega = (r_1, r_2)$ with $-\infty \leqslant r_1 \leqslant r_2 \leqslant \infty$.

We assume the function $\rho: \Omega \to \mathbb{R}$ to be strictly positive and absolutely continuous with derivative $\rho' \in L^2_{\mathrm{loc}}(\Omega; dx)$. Then, using the boundary classification of Feller (cf., e.g., [13, 18]) we get the following results,

r_2 \ r_1		Regular	Exit	Natural	Entrance: Strong	Entrance: Weak
Regular		–	–	–	–	–
Exit		–	+	+	+	–
Natural		–	+	+	+	–
Entrance	Strong	–	+	+	+	–
	Weak	–	–	–	–	–

where "–" means "A is not essentially self-adjoint" and "+" means "A is essentially self-adjoint."

The third section deals with the multidimensional case. It will be restricted to the case $\Omega = \mathbb{R}^n$ $(n \in \mathbb{N})$; i.e., we study the essential self-adjointness of the generalized Schrödinger operator in the Hilbert space $L^2(\mathbb{R}^n; \rho\, dx)$. Our result follows.

If the function $\rho: \mathbb{R}^n \to \mathbb{R}$ is strictly positive and locally Lipschitz continuous, then the operator A with domain $\mathscr{D}(A) = \mathscr{C}_0^\infty(\mathbb{R}^n)$ is essentially self-adjoint in $L^2(\mathbb{R}^n; \rho\, dx)$.

1. A General Criterion for the Essential Self-Adjointness of A

The notation of this section is essentially taken from Fukushima [9]. We recall some basic definitions: Let X be a locally compact, second countable

Hausdorff space and let m be a positive Radon measure on X with $X = \operatorname{supp} m$ (i.e., the support of m). $L^2(X; m)$ denotes the space of all (classes of) m-square integrable, real functions on X with inner product

$$(f, g) = \int_X f(x)\, g(x)\, m(dx) \qquad (f, g \in L^2(X; m)).$$

Let $\mathscr{E}$ be a symmetric form on $L^2(X; m)$ (in the sense of [9]), i.e., $\mathscr{E}$ is a nonnegative definite, symmetric, bilinear form on $L^2(X; m)$ with domain $\mathscr{D}(\mathscr{E})$, where $\mathscr{D}(\mathscr{E})$ is a dense linear subspace of $L^2(X; m)$.

$\mathscr{E}$ is said to be closed, if the space $\mathscr{D}(\mathscr{E})$ is complete with respect to the inner product

$$\mathscr{E}_1(f, g) := \mathscr{E}(f, g) + (f, g) \qquad (f, g \in \mathscr{D}(\mathscr{E})).$$

We say that $\mathscr{E}$ is closable, if the following condition is satisfied:

> Given a sequence $(f_n)_{n \in \mathbb{N}}$ in $\mathscr{D}(\mathscr{E})$ such that $\mathscr{E}(f_n - f_k, f_n - f_k) \to_{n,k \to \infty} 0$ (i.e., $(f_n)_{n \in \mathbb{N}}$ is an $\mathscr{E}$-Cauchy sequence) and $(f_n, f_n) \to_{n \to \infty} 0$, then $\mathscr{E}(f_n, f_n) \to_{n \to \infty} 0$.

Given two symmetric forms $\mathscr{E}^{(1)}$ and $\mathscr{E}^{(2)}$ on $L^2(X; m)$, $\mathscr{E}^{(2)}$ is called an extension of $\mathscr{E}^{(1)}$, if

$$\mathscr{D}(\mathscr{E}^{(1)}) \subset \mathscr{D}(\mathscr{E}^{(2)})$$

and

$$\mathscr{E}^{(2)} = \mathscr{E}^{(1)} \qquad \text{on} \quad \mathscr{D}(\mathscr{E}^{(1)}) \times \mathscr{D}(\mathscr{E}^{(1)}).$$

Clearly a symmetric form on $L^2(X; m)$ is closable, iff there exists a closed extension.

Let $\mathscr{E}$ be a cloable symmetric form. The smallest closed extension of $\mathscr{E}$ with respect to the $\mathscr{E}_1$-metric is called the closure $\bar{\mathscr{E}}$ of $\mathscr{E}$.

There is a well-known correspondence between nonnegative definite, self-adjoint operators H in $L^2(X, m)$ and closed symmetric forms $\mathscr{E}$ on $L^2(X; m)$ (cf. [9]). This correspondence is given by

$$\begin{aligned} &\mathscr{D}(\mathscr{E}) = \mathscr{D}(\sqrt{H}), \\ &\mathscr{E}(f, g) = (\sqrt{H} f, \sqrt{H} g) \qquad (f, g \in \mathscr{D}(\mathscr{E})). \end{aligned} \tag{1.1}$$

We use this correspondence to find self-adjoint extensions of the operator A.

Let Ω be a domain in $\mathbb{R}^n$. $\mathscr{C}_0^\infty(\Omega)$ denotes the set of all infinitely differentiable functions on Ω with compact support in Ω.

Let $\rho: \Omega \to \mathbb{R}$ be a function with the properties (0.2). We are interested in the symmetric form associated with the generalized Schrödinger operator; i.e.,

$$\mathscr{D}(\mathscr{E}) = \mathscr{D}(A) = C_0^\infty(\Omega),$$
$$\mathscr{E}(f, g) = (Af, g) = \frac{1}{2} \sum_{i=1}^{n} \int_\Omega D_i f(x)\, D_i g(x)\, \rho(x)\, dx \qquad (f, g \in \mathscr{D}(\mathscr{E})). \tag{1.2}$$

The following theorem establishes the closability of the form $\mathscr{E}$. We remark that the expression (1.2) already makes sense if $\rho \in L^1_{\mathrm{loc}}(\Omega; dx)$. Sufficient conditions for the closability of this more general symmetric form can be found in [20] (and in the references therein).

1.1. THEOREM. *The form $(\mathscr{D}(\mathscr{E}), \mathscr{E})$ defined in (1.2) is a closable symmetric form on $L^2(\Omega; \rho\, dx)$. Let $(\mathscr{H}_0^{1,2}(\Omega; \rho\, dx), D)$ be the closure of $(\mathscr{D}(\mathscr{E}), \mathscr{E})$ and let H_0 be the associated self-adjoint operator. Then, H_0 is a self-adjoint extension of A.*

Proof. Since the form (1.2) is defined by a symmetric operator, it is closable (cf. [20]). The second assertion follows immediately using (1.1). ∎

Remark. $(\mathscr{H}_0^{1,2}(\Omega; \rho\, dx), D)$ is a regular, local Dirichlet form on $L^2(\Omega; \rho\, dx)$ ([9]). Hence, it admits a symmetric diffusion process on Ω, uniquely in a certain sense ([9, 22]). This process is called the distorted Brownian motion ([4, 10]).

Let $\mathscr{A}(A)$ be the set of all nonnegative definite, self-adjoint extensions of A.

Remark. Introducing a semiorder $<$ in $\mathscr{A}(A)$ by

$$H_1 < H_2 :\Leftrightarrow \mathscr{D}(\mathscr{E}_{H_1}) \subset \mathscr{D}(\mathscr{E}_{H_2}), \qquad \mathscr{E}_{H_1}(f, f) = \mathscr{E}_{H_2}(f, f) \qquad \forall f \in \mathscr{D}(\mathscr{E}_{H_1}),$$

where $\mathscr{E}_{H_i}$ denotes the closed symmetric form corresponding to the self-adjoint operator H_i by (1.1), we can conclude that H_0 is the minimum element of $\mathscr{A}(A)$ according to $<$.

To find other elements of $\mathscr{A}(A)$ we assume further

$$\rho^{-1} \in L^1_{\mathrm{loc}}(\Omega; dx). \tag{1.3}$$

Then Hölder's inequality implies that every $f \in L^2(\Omega; \rho\, dx)$ is locally integrable with respect to the Lebesgue measure on Ω.

Consider the symmetric form defined by

$$\mathscr{D}(\mathscr{E}) = \mathscr{H}^{1,2}(\Omega; \rho\, dx) := \{f \in L^2(\Omega; \rho\, dx) \mid f \text{ is weakly differentiable and } D_i f \in L^2(\Omega; \rho\, dx) \text{ for } 1 \leqslant i \leqslant n\},$$

$$\mathscr{E}(f, g) = D(f, g) = \frac{1}{2} \sum_{i=1}^{n} \int_\Omega D_i f(x)\, D_i g(x)\, \rho(x)\, dx \qquad (f, g \in \mathscr{D}(E)).$$

1.2. THEOREM. *The form* $(\mathscr{H}^{1,2}(\Omega; \rho\, dx), D)$ *is a closed symmetric form on* $L^2(\Omega; \rho\, dx)$. *Let* H_1 *be the associated self-adjoint operator. Then* $H_1 \in \mathscr{A}(A)$.

Proof. First we show the closedness of the form (cf. [20]). Let $(f_n)_{n \in \mathbb{N}}$ be an $\mathscr{E}_1$-Cauchy sequence in $\mathscr{H}^{1,2}(\Omega; \rho\, dx)$. Then there exists functions $f \in L^2(\Omega; \rho\, dx)$ and $h_i \in L^2(\Omega; \rho\, dx)$ $(1 \leqslant i \leqslant n)$ such that

$$\lim_{n \to \infty} f_n = f \qquad \text{in} \quad L^2(\Omega; \rho\, dx)$$

and

$$\lim_{n \to \infty} D_i f_n = h_i \qquad \text{in} \quad L^2(\Omega; \rho\, dx) \qquad (1 \leqslant i \leqslant n).$$

It remains to show that f is weakly differentiable and that $D_i f = h_i$ for $1 \leqslant i \leqslant n$. Let $g \in \mathscr{C}_0^\infty(\Omega)$. Applying Hölder's inequality we obtain for $1 \leqslant i \leqslant n$

$$\left| \int_\Omega (h_i - D_i f_n)\, g\, dx \right| \leqslant \left(\int_\Omega (h_i - D_i f_n)^2\, \rho\, dx \right)^{1/2} \left(\int_\Omega g^2 \rho^{-1}\, dx \right)^{1/2}$$

and

$$\left| \int_\Omega (f - f_n)\, D_i g\, dx \right| \leqslant \left(\int_\Omega (f - f_n)^2\, \rho\, dx \right)^{1/2} \left(\int_\Omega (D_i g)^2\, \rho^{-1}\, dx \right)^{1/2}.$$

It follows that

$$\begin{aligned} \int_\Omega h_i g\, dx &= \lim_{n \to \infty} \int_\Omega (D_i f_n)\, g\, dx \\ &= -\lim_{n \to \infty} \int_n f_n D_i g\, dx \\ &= -\int_\Omega f D_i g\, dx. \end{aligned}$$

To show the second assertion take $u \in \mathscr{D}(H_1)$. Let $(G_\alpha \mid \alpha > 0)$ be the strongly continuous resolvent corresponding to H_1 (cf. [9]). By [9, Lemma 1.3.3] there exists a function $f \in L^2(\Omega; \rho\, dx)$, such that $u = G_\alpha f$ and

$$\alpha(u, g) + D(u, g) = (f, g) \qquad \forall g \in \mathscr{H}^{1,2}(\Omega; \rho\, dx).$$

By partial integration we obtain for all $g \in \mathscr{C}_0^\infty(\Omega)$:

$$\int_\Omega u \left(\alpha g - \frac{1}{2} \frac{\nabla \rho}{\rho} \cdot \nabla g - \frac{1}{2} \Delta g\right) \rho\, dx = \int_\Omega f g \rho\, dx.$$

Therefore $H_1 \subset A^*$ and hence $A \subset H_1$. ∎

Remark. The form $(\mathscr{H}^{1,2}(\Omega; \rho\, dx), D)$ is a local Dirichlet form on $L^2(\Omega; \rho\, dx)$. But in contrast with the form $(\mathscr{H}_0^{1,2}(\Omega; \rho\, dx)\, D)$ it is not regular in general (cf. [9, Example 1.2.3]).

As a necessary condition for the essential self-adjointness of A the self-adjoint extensions H_0 and H_1 must be the same; i.e., the closed symmetric forms $(\mathscr{H}^{1,2}(\Omega; \rho\, dx), D)$ and $(\mathscr{H}_0^{1,2}(\Omega; \rho\, dx), D)$ must coincide. This condition, however, is not sufficient. We have the following theorem:

1.3. THEOREM. *Let $\rho: \Omega \to \mathbb{R}$ be a function with the properties* (0.2) *and* (1.3). *The operator A is essentially self-adjoint in $L^2(\Omega; \rho\, dx)$, iff*

(i) $\mathscr{H}_0^{1,2}(\Omega; \rho\, dx) = \mathscr{H}^{1,2}(\Omega; \rho\, dx)$,

(ii) $\operatorname{Ker}(A^* + \alpha) \subset \mathscr{H}^{1,2}(\Omega; \rho\, dx)$ *for any* $\alpha > 0$.

Proof. Let D_1 be the symmetric form $D_1(f, g) = (f, g) + D(f, g)$ $(f, g \in \mathscr{H}^{1,2}(\Omega; \rho\, dx))$, then $(\mathscr{H}^{1,2}(\Omega; \rho\, dx), D_1)$ is a Hilbert space. By [9, Lemma 2.3.2], it can be orthogonally decomposed as

$$\mathscr{H}^{1,2}(\Omega; \rho\, dx) = \mathscr{H}_0^{1,2}(\Omega; \rho\, dx) \oplus (\operatorname{Ker}(A^* + \alpha) \cap \mathscr{H}^{1,2}(\Omega; \rho\, dx)) \ (\alpha > 0).$$

Hence, we obtain $\operatorname{Ker}(A^* + \alpha) = \{0\}$ for any $\alpha > 0$ iff the conditions (i) and (ii) are satisfied; thus the assertion follows by (0.3). ∎

Remark. Examples, where the condition (i) of Theorem 1.3 holds, can be found, e.g., in [16, 25]. On the other hand, it is easy to give examples, where this condition is not satisfied, so that in these cases the operator A is not essentially self-adjoint:

EXAMPLE. Let Ω be a bounded domain in $\mathbb{R}^n$. Let $\rho: \Omega \to \mathbb{R}$ be a function that satisfies conditions (0.2) and (1.3). We assume that there are constants c_1, c_2 such that for almost all $x \in \Omega$

$$0 < c_1 \leqslant \rho(x) \leqslant c_2 < \infty.$$

Then by Poincaré's inequality there exists a constant c depending only on ρ and Ω such that for all $f \in \mathscr{H}_0^{1,2}(\Omega; \rho\, dx)$

$$(f, f) \leqslant c \sum_{i=1}^{n} (D_i f, D_i f).$$

Hence, the function $f \equiv 1$ is not contained in $\mathscr{H}_0^{1,2}(\Omega; \rho\, dx)$. This implies $\mathscr{H}_0^{1,2}(\Omega; \rho\, dx) \neq \mathscr{H}^{1,2}(\Omega; \rho\, dx)$. Thus A is not essentially self-adjoint in this case.

2. The One-Dimensional Case

Let Ω be the open interval (r_1, r_2), where $-\infty \leqslant r_1 < r_2 \leqslant \infty$. Let $\rho: \Omega \to \mathbb{R}$ be a function that satisfies the following conditions:

$$\begin{aligned} &\rho \text{ is strictly positive,} \\ &\rho \text{ is absolutely continuous,} \\ &\rho' \in L^2_{\mathrm{loc}}(\Omega; \rho\, dx). \end{aligned} \tag{2.1}$$

Then ρ has properties (0.2) and (1.3). Using partial integration it is easy to show that the adjoint operator A^* is given by

$$A^* f = Lf = -\frac{1}{2} \frac{1}{\rho} (\rho f')',$$

$$\mathscr{D}(A^*) = \{f \in L^2(\Omega; \rho\, dx) \mid f \text{ is continuously differentiable on } \Omega,$$
$$f' \text{ is absolutely continuous, } Lf \in L^2(\Omega; \rho\, dx)\}.$$

Before starting with the calculation of the set $\operatorname{Ker}(A^* + \alpha)$, according to the criterion (0.3), we discuss some technical preliminaries taken from the theory of differential equations (cf., e.g. [18]).

Let $\alpha > 0$.

Definition. A function $g: \Omega \to \mathbb{R}$ is called a solution of the equation $(L + \alpha) g = 0$, if

$$\begin{aligned} &g \text{ is continuously differentiable,} \\ &g' \text{ is absolutely continuous,} \\ &\tfrac{1}{2}(\rho g')' = \alpha \rho g \text{ a.e. in } \Omega. \end{aligned}$$

Let c be a real point such that $r_1 < c < r_2$. Set for $n \in \mathbb{N}_0$, $x \in \Omega$,

$$u_0 = 1, \qquad u_{n+1}(x) = \int_c^x \left(\int_c^y u_n(t)\,\rho(t)\,dt \right) \frac{1}{\rho(y)}\,dy.$$

Then each function u_n is continuously differentiable and the following inequalities hold for all $x \in \Omega$ and $n \in \mathbb{N}_0$:

$$\begin{aligned} u_n(x) &\leqslant \frac{(u_1(x))^n}{n!}, \\ |\rho(x)\,u'_{n+1}(x)| &\leqslant \left| \int_c^x \rho(t)\,dt \right| \frac{(v_1(x))^n}{n!}, \end{aligned} \tag{2.2}$$

where $v_1(x) := \int_c^x (\int_c^y (1/\rho(t))\,dt)\,\rho(y)\,dy$. Denote $w(x) := \sum_{n=0}^{\infty} (2\alpha)^n u_n(x)$. It follows from (2.2) that this series converges and that for all $x \in \Omega$

$$\begin{gathered} 1 + 2\alpha u_1(x) \leqslant w(x) \leqslant \exp(2\alpha u_1(x)), \\ 2\alpha \left| \int_c^x \rho(y)\,dy \right| \leqslant |\rho(x)\,w'(x)| \leqslant 2\alpha \left| \int_c^x \rho(t)\,dt \right| \exp(2\alpha v_1(x)). \end{gathered} \tag{2.3}$$

Let us introduce the functions

$$\begin{aligned} w_0(x) &:= w(x) \int_c^x \frac{1}{w^2(y)\,\rho(y)}\,dy, \\ w_1(x) &:= w(x) \int_{r_1}^x \frac{1}{w^2(y)\,\rho(y)}\,dy, \\ w_2(x) &:= w(x) \int_x^{r_2} \frac{1}{w^2(y)\,\rho(y)}\,dy. \end{aligned}$$

These functions are well-defined, because

$$\int_{r_1}^{r_2} \frac{1}{w^2(y)\,\rho(y)}\,dy < \infty.$$

w_1 and w_2 are positive functions, w_1 is increasing while w_2 is decreasing.

2.1. THEOREM. *The functions w, w_0, w_1, w_2 are solutions of the equation $(L + \alpha)\,g = 0$. Each solution of this equation is a linear combination of two of these functions.*

Proof. The first assertion follows by an easy computation, the second by standard arguments taken from the theory of differential equations (cf. [18]). ∎

2.2. LEMMA. *Let f be a non-trivial solution of the equation $(L+\alpha)g=0$. For all d_1, d_2 such that $r_1 < d_1 < c < d_2 < r_2$, there exists a constant $k = k(f, d_1, d_2) > 0$, such that*

$$\int_{r_1}^{r_2} f^2(x)\,\rho(x)\,dx \geqslant k \cdot \min\left\{\int_{d_2}^{r_2} w^2(x)\,\rho(x)\,dx, \int_{r_1}^{d_1} w^2(x)\,\rho(x)\,dx\right\}.$$

Proof. By Theorem 2.1 there exist constans $c_1, c_2 \in \mathbb{R}$, such that for all $x \in \Omega$

$$f(x) = c_1 w(x) + c_2 w_0(x).$$

Take $d_1, d_2 \in \mathbb{R}$ such that $r_1 < d_1 < c < d_2 < r_2$. If $c_1 \neq 0$, $c_2 = 0$ or $c_1 > 0$, $c_2 > 0$ or $c_1 < 0$, $c_2 < 0$ we get

$$\int_{r_1}^{r_2} f^2(x)\,\rho(x)\,dx \geqslant \int_{d_2}^{r_2} f^2(x)\,\rho(x)\,dx \geqslant c_1^2 \int_{d_2}^{r_2} w^2(x)\,\rho(x)\,dx.$$

If $c_1 = 0$, $c_2 \neq 0$ it follows

$$\int_{r_1}^{r_2} f^2(x)\,\rho(x)\,dx \geqslant c_2^2 \left(\int_c^{d_2} \frac{1}{w^2(y)\,\rho(y)}\,dy\right)^2 \int_{d_2}^{r_2} w^2(x)\,\rho(x)\,dx.$$

If $c_1 < 0$, $c_2 > 0$ or $c_1 > 0$, $c_2 < 0$ we obtain

$$\begin{aligned}\int_{r_1}^{r_1} f^2(x)\,\rho(x)\,dx &\geqslant \int_{r_1}^{d_1} f^2(x)\,\rho(x)\,dx\\ &= \int_{r_1}^{d_1} w^2(x)\left[c_1 - c_2\int_x^c \frac{1}{w^2(y)\,\rho(y)}\,dy\right]^2 \rho(x)\,dx\\ &\geqslant c_1^2 \int_{r_1}^{d_1} w^2(x)\,\rho(x)\,dx. \quad \blacksquare\end{aligned}$$

In the next theorem we consider the case $\Omega = \mathbb{R}$.

2.3. THEOREM. *Under the assumptions* (2.1) *the operator A is essentially self-adjoint in $L^2(\mathbb{R}; \rho\,dx)$.*

Proof. Take $d_1, d_2 \in \mathbb{R}$ such that $-\infty < d_1 < c < d_2 < \infty$. Hölder's inequality implies

$$\infty = \int_{-\infty}^{d_1} \frac{1}{w^2(y)\,\rho(y)}\,dy \int_{-\infty}^{d_1} w^2(y)\,\rho(y)\,dy$$

and

$$\infty = \int_{d_2}^{\infty} \frac{1}{w^2(y)\rho(y)}\,dy \int_{d_2}^{\infty} w^2(y)\rho(y)\,dy.$$

Since $\int_{-\infty}^{\infty} (1/w^2(y)\rho(y))\,dy < \infty$, we obtain

$$\infty = \int_{d_2}^{\infty} w^2(y)\rho(y)\,dy = \int_{-\infty}^{d_1} w^2(y)\rho(y)\,dy.$$

Hence by Lemma 2.2 the trivial solution is the only L^2-solution of the equation $(L+\alpha)g = 0$ and the assertion follows by (0.3). ∎

To determine the set $\operatorname{Ker}(A^* + \alpha)$ in the case $\Omega \neq \mathbb{R}$ we classify the boundaries r_1, r_2 according to the behaviour of the functions $m(x) := \int_c^x \rho(t)\,dt$ and $s(x) := \int_c^x (1/\rho(t))\,dt$ in their neighborhoods. Let us first recall the definitions of the functions u_1 and v_1:

$$u_1(x) := \int_c^x \left(\int_c^y \rho(t)\,dt\right) \frac{1}{\rho(y)}\,dy,$$

$$v_1(x) := \int_c^x \left(\int_c^y \frac{1}{\rho(t)}\,dt\right) \rho(y)\,dy.$$

For the rest of this section, let $i, j \in \{1, 2\}$ with $i \neq j$.

Definition. r_i is called an accessible boundary if $u_1(r_i) < \infty$.
r_i is called an inaccessible boundary if $u_1(r_i) = \infty$.
An accessible boundary r_i is called regular if $v_1(r_i) < \infty$.
An accessible boundary r_i is called an exit boundary if $v_1(r_i) = \infty$.
An inaccessible boundary r_i is called an entrance boundary if $v_1(r_i) < \infty$.
An inaccessible boundary r_i is called a natural boundary if $v_1(r_i) = \infty$.

The names of the boundaries are in accordance with the behaviour of the diffusion processes associated with A. The function m is called the speed of the process, the function s is called the scale of the process (cf. [13]). For related work on the analytical treatment of one-dimensional diffusions see [18, 21].

It is easy to check that r_i is regular iff both $m(r_i)$ and $s(r_i)$ are finite. If r_i is an entrance boundary, then $m(r_i)$ is finite but $s(r_i) = \pm\infty$. If r_i is an exit boundary, then $s(r_i)$ is finite but $m(r_i) = \pm\infty$.

2.4. Examples. (1) Let $\rho: \mathbb{R} \to \mathbb{R}$ be the function $\rho(x) = \exp(|x|^{2+\varepsilon})$ with $\varepsilon \geqslant -1$. The points $+\infty$ and $-\infty$ are

(i) natural boundaries if $-1 \leqslant \varepsilon \leqslant 0$,

(ii) exit boundaries if $\varepsilon > 0$.

(2) Let ρ: $(0, b) \to \mathbb{R} (b > 0)$ be the function $\rho(x) = x^{\varepsilon}$ with $\varepsilon \in \mathbb{R}$. The point 0 is

(i) an entrance boundary if $\varepsilon \geqslant 1$,
(ii) a regular boundary if $|\varepsilon| < 1$,
(iii) an exit boundary if $\varepsilon \leqslant -1$.

The boundary behaviour of w_1 and w_2 is summarized in the table ([13, 21])

r_i	Regular	Exit	Entrance	Natural
$w_i(r_i)$	$=0$	$=0$	>0	$=0$
$w_j(r_i)$	$<\infty$	$<\infty$	$=\infty$	$=\infty$
$\rho(r_i)\, w_i'(r_i)$	>0	>0	$=0$	$=0$
$\rho(r_i)\, w_j'(r_i)$	$<\infty$	$=\infty$	$<\infty$	$=\infty$

2.5. LEMMA. *For all $d_1, d_2 \in \mathbb{R}$ such that $r_1 < d_1 < c < d_2 < r_2$, there exists a constant $k = k(d_1, d_2) > 0$, such that*

$$\int_{d_2}^{r_2} w^2(x)\,\rho(x)\,dx \geqslant k \int_{d_2}^{r_2} \left(\int_{d_2}^{x} \frac{1}{\rho(y)}\,dy\right)^2 \rho(x)\,dx,$$

$$\int_{r_1}^{d_2} w^2(x)\,\rho(x)\,dx \geqslant k \int_{r_1}^{d_1} \left(\int_{x}^{d_1} \frac{1}{\rho(y)}\,dy\right)^2 \rho(x)\,dx.$$

Proof. Take $d_1, d_2 \in \mathbb{R}$ such that $r_1 < d_1 < c < d_2 < r_2$. Then

$$\begin{aligned}\int_{d_2}^{r_2} w^2(x)\,\rho(x)\,dx &\geqslant (2\alpha)^2 \int_{d_2}^{r_2} u_1^2(x)\,\rho(x)\,dx \\ &\geqslant (2\alpha)^2 \int_{d_2}^{r_2} \left[\int_{d_2}^{x} \left(\int_{c}^{y} \rho(t)\,dt\right) \frac{1}{\rho(y)}\,dy\right]^2 \rho(x)\,dx \\ &\geqslant \left[2\alpha \int_{c}^{d_2} \rho(t)\,dt\right]^2 \int_{d_2}^{r_2} \left(\int_{d_2}^{x} \frac{1}{\rho(y)}\,dy\right)^2 \rho(x)\,dx.\end{aligned}$$

Similarly

$$\begin{aligned}&\int_{r_1}^{d_1} w^2(x)\,\rho(x)\,dx \\ &\qquad \geqslant \left[2\alpha \int_{d_1}^{c} \rho(t)\,dt\right]^2 \int_{r_1}^{d_1} \left(\int_{x}^{d_1} \frac{1}{\rho(y)}\,dy\right)^2 \rho(x)\,dx. \quad \blacksquare\end{aligned}$$

2.6. THEOREM. *Let $i, j \in \{1, 2\}$, $i \neq j$. Then we have*

(a) $|\int_c^{r_i} w_i^2(x)\,\rho(x)\,dx| < \infty$.

(b) *If r_i is a regular boundary, then* $|\int_c^{r_i} w_j^2(x)\,\rho(x)\,dx| < \infty$.

(c) *If r_i is an exit boundary, then* $|\int_c^{r_i} w^2(x)\,\rho(x)\,dx| = \infty$.

(d) *If r_i is a natural boundary, then* $|\int_c^{r_i} w^2(x)\,\rho(x)\,dx| = \infty$.

Proof. (a) We have $|\int_c^{r_i} w_i(x)\,\rho(x)\,dx| < \infty$, because

$$\begin{aligned} 2\alpha \int_c^{r_i} w_i(x)\,\rho(x)\,dx &= \int_c^{r_i} (w_i'(x)\,\rho(x))'\,dx \\ &= w_i'(r_i)\,\rho(r_i) - w_i'(c)\,\rho(c). \end{aligned}$$

Since w_i is monotonous we get

$$\left| \int_c^{r_i} w_i^2(x)\,\rho(x)\,dx \right| \leqslant w_i(c) \left| \int_c^{r_i} w_i(x)\,\rho(x)\,dx \right| < \infty.$$

(b) Since r_i is regular, r_i is finite. Hence the assertion follows, because the functions ρ and w are continuous.

(c) This assertion follows from the inequality

$$\left| \int_c^{r_i} w^2(x)\,\rho(x)\,dx \right| \geqslant \left| \int_c^{r_i} \rho(x)\,dx \right| = \infty.$$

(d) By Lemma 2.5 we obtain

$$\left| \int_c^{r_i} w^2(x)\,\rho(x)\,dx \right| \geqslant k' v_1(r_i) = \infty. \quad \blacksquare$$

2.7. THEOREM. *If r_i is an entrance boundary, then there exist constants k_1, k_2 such that*

$$\left| \int_c^{r_i} w^2(x)\,\rho(x)\,dx \right| \leqslant k_1 + k_2 \left| \int_c^{r_i} \left(\int_c^x \frac{1}{\rho(y)}\,dy \right)^2 \rho(x)\,dx \right|.$$

Proof. Let r_i be an entrance boundary, then $|\int_c^{r_i} w(x)\,\rho(x)\,dx| < \infty$, because we obtain by the inequality (2.3)

$$\begin{aligned} (2\alpha) \left| \int_c^{r_i} w(x)\,\rho(x)\,dx \right| &= \left| \int_c^{r_i} (w'(x)\,\rho(x))'\,dx \right| \\ &= |w'(r_i)\,\rho(r_i)| \\ &\leqslant (2\alpha) \left| \int_c^{r_i} \rho(t)\,dt \right| \exp(2\alpha v_1(r_i)) \\ &< \infty. \end{aligned}$$

Integrating the equation $(1/2)(1/\rho)(\rho w')' = \alpha w$ twice, we get for all $x \in \Omega$

$$w(x) = 1 + 2\alpha \int_c^x \frac{1}{\rho(y)} \left(\int_c^y w(t)\,\rho(t)\,dt \right) dy.$$

Hence

$$\left| \int_c^{r_i} w^2(x)\,\rho(x)\,dx \right|$$

$$\leqslant 2 \left| \int_c^{r_i} \rho(x)\,dx \right| + 8\alpha^2 \left| \int_c^{r_i} w(t)\,\rho(t)\,dt \right|^2 \int_c^{r_i} \left(\int_c^x \frac{1}{\rho(y)}\,dy \right)^2 \rho(x)\,dx. \quad \blacksquare$$

DEFINITION. Let r_i be an entrance boundary. We call r_i a strong entrance boundary, if

$$\left| \int_c^{r_i} \left(\int_c^x \frac{1}{\rho(y)}\,dy \right)^2 \rho(x)\,dx \right| = \infty.$$

r_i is called a weak entrance boundary, if

$$\left| \int_c^{r_i} \left(\int_c^x \frac{1}{\rho(t)}\,dt \right)^2 \rho(x)\,dx \right| < \infty.$$

2.8. COROLLARY. *Let r_i be an entrance boundary.*

(a) *If r_i is a weak entrance boundary, then $|\int_c^{r_i} w_j^2(x)\,\rho(x)\,dx| < \infty$.*

(b) *If r_i is a strong entrance boundary, then $|\int_c^{r_i} w^2(x)\,\rho(x)\,dx| = \infty$.*

Proof. The second assertion follows with Lemma 2.5, the first from the inequality

$$\left| \int_c^{r_i} w_j^2(x)\,\rho(x)\,dx \right| \leqslant \left| \int_{r_j}^{r_i} \frac{1}{w^2(y)\,\rho(x)}\,dy \right|^2 \left| \int_c^{r_i} w^2(x)\,\rho(x)\,dx \right| . \quad \blacksquare$$

We know that the operator A is essentially self-adjoint iff the trivial solution is the only L^2-solution of the equation $(L + \alpha) g = 0$ (cf. (0.3)). Hence, applying the results of the last theorems, we get the table

r_2 \ r_1		Regular	Exit	Natural	Entrance: Strong	Entrance: Weak
Regular		−	−	−	−	−
Exit		−	+	+	+	−
Natural		−	+	+	+	−
Entrance	Strong	−	+	+	+	−
	Weak	−	−	−	−	−

where "$-$" means that "A is not essentially self-adjoint" and "$+$" means that "A is essentially self-adjoint."

2.9. EXAMPLE. Let $\rho: \mathbb{R} \to \mathbb{R}$ be the function $\rho(x) = \exp(2|x|)$. Then ρ is strictly positive, absolutely continuous with $\rho' \in L^2_{\mathrm{loc}}(\mathbb{R}; dx)$. The points $-\infty$ and $+\infty$ are natural boundaries (see Example 2.4 (1)). Hence the operator A is essentially self-adjoint in $L^2(\mathbb{R}; \rho\, dx)$.

This implies in particular, that the Schrödinger operator $H = \phi A \phi^{-1}$ as defined in (0.1) is essentially self-adjoint in $L^2(\mathbb{R}; dx)$ on the domain $\mathscr{D}(H) = \phi \mathscr{D}(A)$. H can be described as $-\frac{1}{2}\Delta + \delta + \frac{1}{2}$ as sum of positive quadratic forms.

Remark. The above table gives general conditions for the essential self-adjointness of A in terms of the boundary behaviour of the function ρ. The nomenclature of the boundaries is in accordance with the behaviour of the stochastic processes associated with the self-adjoint extensions of A. In particular, the essential self-adjointness of A is a sufficient condition to get a unique process (modulo equivalence). This condition, however, is not necessary (cf. [10, 26]).

Uniqueness problems and more general boundary behaviour of processes have been discussed in the probabilistic literature, see, e.g. [7, 13, 18, 23].

3. THE MULTIDIMENSIONAL CASE

Now we treat the case, where $\Omega = \mathbb{R}^n$ and $n \in \mathbb{N}$. We recall that a function $g: \mathbb{R}^n \to \mathbb{R}$ is locally Lipschitz continuous, if for every compact set $K \subset \mathbb{R}^n$ there exists a constant $c_K > 0$ such that for all $x, y \in K$ $|g(x) - g(y)| \leqslant c_K |x - y|$. A locally Lipschitz continuous function has the properties (0.2) and (1.3). The idea of the proof of the following theorem is essentially taken from [14, V, Section 3.7].

3.1. THEOREM. *Let the function $\rho: \mathbb{R}^n \to \mathbb{R}$ be strictly positive and locally Lipschitz continuous. Then, the operator A is essentially self-adjoint in the Hilbert space $L^2(\mathbb{R}^n; \rho\, dx)$.*

Proof. According to (0.3) it suffices to show that for an $\alpha > 0$ the trivial solution is the only L^2-solution of the equation $(A^* + \alpha) g = 0$.

Take an $\alpha > 0$. Let $g \in L^2(\mathbb{R}^n; \rho\, dx)$ be a function such that for all $f \in \mathscr{C}_0^\infty(\mathbb{R}^n)$

$$(g, (A + \alpha) f) = 0.$$

Then by [8, Theorem 2.1], g is twice weakly differentiable, and the weak derivatives are $L^2_{\mathrm{loc}}(\mathbb{R}^n; \rho\, dx)$-functions. It is easy to show that for all $\varphi \in \mathscr{C}_0^\infty(\mathbb{R}^n)$

$$\varphi \cdot g \in \mathscr{D}(\overline{A+\alpha}), \qquad \text{where } \overline{A+\alpha} \text{ denotes the closure of the operator } A+\alpha.$$

Partial integration leads to the inequality

$$(\varphi \cdot g, (\overline{A+\alpha})\, \varphi \cdot g) = \frac{1}{2} \sum_{i=1}^{n} ((D_i \varphi) g, (D_i \varphi) g).$$

On the other hand, we get for all $\varphi \in \mathscr{C}_0^\infty(\mathbb{R}^n)$

$$(\varphi \cdot g, (\overline{A+\alpha})\varphi \cdot g) \geqslant \alpha(\varphi \cdot g, \varphi \cdot g).$$

Hence, the following inequality holds for all $\varphi \in \mathscr{C}_0^\infty(\mathbb{R}^n)$

$$\alpha(\varphi \cdot g, \varphi \cdot g) \leqslant \frac{1}{2} \sum_{i=1}^{n} ((D_i \varphi) g, (D_i \varphi) g). \tag{3.1}$$

Now, we take a sequence $(\varphi_m)_{m \in \mathbb{N}}$ of functions $\varphi_m \in \mathscr{C}_0^\infty(\mathbb{R}^n)$ with the properties

$$\begin{aligned} \varphi_m(x) &= 1 && \text{for} \quad |x| \leqslant m, \\ \varphi_m(x) &= 0 && \text{for} \quad |x| \geqslant m+1, \\ 0 \leqslant \varphi_m &\leqslant 1 && \text{for all } m \in \mathbb{N}, \\ \sup_{1 \leqslant i \leqslant n} \sup_{x \in \mathbb{R}^n} |D_i \varphi_m(x)| &< M && \text{for all } m \in \mathbb{N} \quad (M > 0). \end{aligned}$$

If we put these functions into inequality (3.1) we obtain for all $m \in \mathbb{N}$

$$0 \leqslant \alpha \int_{|x|<m} g^2(x)\, \rho(x)\, dx \leqslant \frac{n}{2} M^2 \int_{|x|>m} g^2(x)\, \rho(x)\, dx.$$

Hence, taking the limit $m \to \infty$, we conclude that g is the trivial functions in $L^2(\mathbb{R}^n; \rho\, dx)$. ∎

Remark. The assumptions of Theorem 3.1 are weaker than the ones in [4, 12]. Besides this, the domain $\mathscr{D}(A)$ of the operator A is different from the one in the cited references. In particular, this theorem yields a new result on the uniqueness question of quantum mechanical dynamics.

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